======= EPODOC =======

TI - Method for the prognosis of inhibitor or toxicological carcinogenic action of organic nitrogen compounds

AB - The invention relates to a method for the prognosis of inhibitor or toxicological carcinogenic action of organic nitrogen compounds, especially aryl amines before the start of chemical synthesis. This prognosis is carried out using a base data set of structures hitherto experimentally evaluated as safe in regard to their action with the use of various pattern-recognition methods such as, for example, fuzzy clustering, primary-component analysis or the use of neuronal networks. In this case, simulation results are accepted only if the same classification results are obtained for the pattern recognition using different characteristic sets and different mathematical models.

PN - DE4309883 A 19940929
AP - DE19934309883 19930326
PR - DE19934309883 19930326
PA - BUNA AG (DE)
IN - EITNER BERND DR (DE); ADLER BERNHARD PROF DR (DE)
EC - G01N33/574 ; C07C211/43 ; C07C211/45 ; C07C211/50 ; C07C211/54
CT - ***** Citations of A -Document: *****
- DE4137220 A1 [ ]
- ***** Citations of C2-Document: *****
- DE4137220 A1 [ ]
CTNP - ***** Citations of A -Document: *****
- [ ] ADLER, B., et.al.: In: Chemische Technik 45, 1993, 2, S.94-98
- ***** Citations of C2-Document: *****
- [ ] ADLER, B., et.al.: In: Chemische Technik 45, 1993, 2, S.94-98
DT - *

======= WPI =======

TI - Mathematical prediction of antioxidant and carcinogenic activity - of organic nitrogen cpds., esp. arylamines.

AB - DE4309883 Method for predicting the inhibitory (antioxidant) and carcinogenic activity of organic N cpds., esp. arylamines, before commencing chemical synthesis comprises: (a) partitioning a learning set of arylamines having known inhibitory and carcinogenic activities into active and inactive structures by a pattern recognition process, e.g. fuzzy clustering, principal component analysis or neural net analysis; (b) using the following descriptor (I) to simulate the inhibitory activity:
- x = (cN, F(5)N, 3X2)
- where CN = a Huckel molecular orbital (HMO) expansion coefft.; F(5)N = an autocorrelation parameter based on inherent electronegativity over five bonds from the N atom; and 3X2 = the connectivity index of three bonds arranged in a star shape; (c) using two different combination descriptors to simulate the carcinogenic activity, where one comprises electro-topological values according to formula (II) and the other comprises the connectivity indices mX1 of substructure elements selected according to formula (III):
- where the sigma values denote the no. of sigma and valence electrons of atoms i and j respectively; rij is the topological distance between atoms i and j; and bj = the bonding of atom j; (d) characterising the simulations in terms of Bayesian statistical parameters; (e) using the results to predict structures that will be non-carcinogenic and have inhibitory activity; and (f) synthesising cpds. with the predicted structures and testing them for mutagenicity.
- ADVANTAGE - The method provides a rapid and inexpensive means of predicting activity to minimise hazards associated with toxicological testing.
- (Dwg.0/7)
PN - DE4309883 A1 19940929 DW199438 G01N33/15 014pp
- DE4309883 C2 19981119 DW199850 G01N33/15 000pp
PR - DE19934309883 19930326
PA - (BUNA) BUNA AG
- (BUNA) BUNA SOW LEUNA OLEFINVERBUND GMBH
IN - ADLER B; EITNER B
MC - E10-B04A1 E10-B04A2 J04-C
- S03-E14A1
DC - E14 E19 J04 S03
IC - G01N33/15
AN - 1994-303837 [38]